Uncertainty Propagation Using Taylor Series Expansion and a Spreadsheet

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ABSTRACT

Most analytical models include variables that have randomness or uncertainties associated with them. These models span many scientific and engineering disciplines. Analyzing these models without incorporating the uncertainties may provide misleading results. In this paper, several methods for evaluating uncertainty are summarized. One of these methods is illustrated using the Lotus 1-2-3 spreadsheet package. In particular, a model's uncertainty is determined by using multivariate Taylor series expansion. Lotus 1-2-3 macros and formulae for Taylor series expansion, along with a worked example, are presented. It is the intent of this paper to provide Idaho researchers with a viable tool for estimating uncertainty for any model that may be evaluated using a spreadsheet.

KEYWORDS

uncertainty analysis

Taylor series expansion

spreadsheet

1. Introduction

Given a formula which models a system, obtaining an answer is usually a relatively simple process which involves evaluating the formula using the estimates for each variable contained within the formula. However, what exactly does the outcome represent? If the formula incorporates variables which have uncertainties (i.e., have a specific distribution or range), the results of the formula must incorporate the variable uncertainty in order to be considered valid. Evaluating models that contain random variables by exclusively using point estimate values does not incorporate the uncertainty of the independent variables and does not provide complete results. This view is widely held in the risk analysis community, and is illustrated by Garlick and Holloway (1987) who state, "Point estimates will be expected, but, however produced, they will lack credibility without clear justification for preferring one value in a range to all the others."

The results from simple formulas with random variables having insignificant uncertainty will be affected minimally by not performing uncertainty analysis. However, for complex systems or models that have random variables with non-negligible uncertainties, ignoring uncertainty may lead to misleading results. Also, without performing the uncertainty analysis, no indicator of the possible range of results is available.

Evaluating the uncertainty of a function of random variables can be accomplished by several different methods using many different analysis tools. For example, Seila and Banks (1990) illustrate a method of performing Monte Carlo simulation using an electronic spreadsheet. In general though, only a couple of different methods of uncertainty analysis are used by analysts. A summary of four of the more popular uncertainty methods appear below.

Sensitivity Analysis This method of uncertainty analysis involves changing a single parameter of the model, requantifying the model to obtain a new result, and then comparing the change in the results versus the change in the parameter. For example, economic models (such as a mortgage payment schedule) are designed so that one of the parameters, such as the interest rate, may be varied so that the monthly payments are analyzed with respect to the varying interest rate. Sensitivity analysis has several different forms, including extreme value analysis where only upper or lower estimates of the parameters are used to quantify the model. These types of sensitivity analyses are simple but suffer from several drawbacks, including:

- The entire model must be requantified each time a parameter is varied. For complex models with many parameters, a comprehensive sensitivity analysis for all of the model variables may be tedious or time consuming. Enhanced sampling approaches (e.g., Latin Hypercube sampling) will help to minimize time impacts.

- The variable parameters may be modified in an arbitrary manner. For the mortgage example above, the interest rate could be changed in increments of 0.25% for several points around the expected interest rate to provide a somewhat comprehensive analysis. But, for other parameters, the choice of values for the sensitivity analysis may not be as straightforward.

- The parameters that are modified for the analysis may be modeled very well by some type of probability distribution (such as lognormal, gamma, normal, etc.). Sensitivity analysis is a point-by-point change, which results in overlooking a parameter's distributional characteristics. While it may be possible to sample input values from the range of the parameter’s distribution, this type of sampling may increase the time needed to perform the analysis.

- Sensitivity analysis lacks coupled variable changes. For a model with many variables, it is reasonable to expect that more than one parameter should be modified at the same time. Also, a model of many variables could have several different probability distributions. The interaction between the distributions are not modeled adequately by changing only one of the model parameters.

If the input variables are statistically correlated, one-at-a-time sensitivity analysis does not address such correlations. While it may be possible to vary more than one parameter at a time, attempting to evaluate all the potential combinations of input parameters may be unmanagable.

Direct Uncertainty Assessment This method of analysis is probably the oldest technique of uncertainty analysis, and can be used to estimate uncertainty on both input parameters and output results. Direct assessment of uncertainty consists of arbitrarily assigning uncertainty bounds on the model in question. For example, a human task analysis model may predict a human error rate of 0.025 per hour. The analyst may conclude that the worst possible error rate is 0.25 per hour, while the most favorable error rate is 0.0025 per hour. While this example is a simple demonstration of direct uncertainty assessment, the actual determination of the uncertainty can sometimes be complicated, and in all cases is conditional on the individual opinions of the analyst. Drawbacks to this type of analysis include:

- The process of selecting uncertainty bounds on the model is very subjective and depends on the viewpoint of the analyst.

- Explaining and defending the rationale that was used in the determination of the uncertainty bounds could be difficult (i.e., the assessment may be based strictly upon "engineering judgement").

- Since the uncertainty is usually based upon the opinion of the analyst, statistical modeling is not incorporated.

Taylor Series Expansion This analysis involves the mathematical evaluation of the model equation. The statistical moments (mean, variance, skewness, etc.) for the model are calculated by expanding the model equation in a Taylor series about the means. What results from the expansion process is an equation for the overall model statistical moments which is a function of the variable moments and the partial derivatives of the model equation. Drawbacks to this type of analysis include:

- Numerical differentiation may be difficult or may be done incorrectly leading to incorrect results.

- The numeric expansion may only be good for functions that are linear or nearly linear (unless many terms are used in the expansion).

- The method is strictly based upon calculations involving a parameter's statistical moments and does not directly incorporate the parameter's probability distribution (e.g., normal, lognormal, gamma). Also, the expansion results only return an estimate of the statistical moments and not a distribution.

- Higher order estimates may be necessary to adequately address highly skewed distributions.

- The model may not be defined explicitly as a function of the input variables. As such, a Taylor expansion about the mean is not possible for these cases.

Monte Carlo Simulation This method of uncertainty analysis may be the most popular method of analysis. Monte Carlo analysis involves sampling the model using the parameters' probability distribution functions to provide parameter values. Usually, a computer-generated random number is used to obtain a parameter value based on the parameter's probability distribution function. When a value for each parameter has been calculated, the model is quantified to obtain an answer. This answer is then placed into a frequency table. The entire process is then repeated until a desired number of iterations is reached. Drawbacks to this type of analysis include:

- Model simulation runtime may be too long for some complex models.

- Calculating numerous parameter values needed for many iterations may be time consuming.

- Failure of the computer-generated random numbers to display randomness may skew the results toward certain values, leaving the resulting statistical parameters suspect. But, in general, modern random number generators do not suffer from this problem.

- Selecting the proper probability distribution function for the model parameters may be difficult in light of inadequate data or a lack of understanding of the underlying physical processes.

In this article, I demonstrate the Taylor series expansion method. Section 2 defines the statistical terms used throughout this article. Section 3 covers the Taylor series expansion development and the techniques used to implement the Taylor series analysis within a spreadsheet environment such as LOTUS 1-2-3 or EXCEL. In Section 4, I demonstrate the uncertainty analysis methodology by examining a sample problem. Section 5 closes the article by presenting uncertainty analysis considerations and conclusions.

2. Uncertainty Analysis Statistical Review

To begin this brief statistical review, the notation used in this paper will be specified. Following the nomenclature, the terms will be defined as needed. This section will address only those topics used in this paper. The statistical notation used is:

μ = mean (first moment) about the origin

σ = standard deviation (square root of variance)

Var = variance (second moment) about the mean

Δ	=	mesh spacing or stepsize
f	=	probability density function (PDF)
g	=	user defined function
m	=	sample mean
s^2	=	sample variance

Taking each item in turn, the mean or first statistical moment for a continuous random variable is defined by (where the integral exists)

$$\mu = \int_{-\infty}^{\infty} x f(x) dx \ . \tag{1}$$

The standard deviation is defined as the square root of the variance, where the variance or second statistical moment is given as (where the integral exists)

$$Var = \sigma^2 = \int_{-\infty}^{\infty} (x - \mu)^2 f(x) dx \ . \tag{2}$$

For the two equations above, the PDF may change depending on the variable in a particular system model. Proper evaluation of the PDF or statistical data for the variables in a model is required in order to obtain the correct mean and standard deviation. But, it is beyond the scope of this paper to discuss issues related to the use and manipulation of PDFs. Frequently, though, the analyst will not need to develop or use a PDF since statistical data may be available. If data is available, the sample mean and standard deviation are available through estimation theory, using the familiar equations

$$m = \frac{1}{N} \sum_{i=1}^{N} X_i \tag{3}$$

$$s^2 = \frac{1}{N-1}\sum_{i=1}^{N}(X_i - m)^2 \ , \qquad \textbf{(4)}$$

where X_i are the specific data points and N is the total number of data points.

3. Taylor Series Expansion Development

Let a system or model, denoted by S, be defined by:

$$S = g(x_1, x_2, \ldots, x_n) \ , \qquad \textbf{(5)}$$

where x_1, x_2,..., x_n are system variables. The system variables can represent any portion of the system but, for the 2nd order analysis presented in this paper, must be mutually statistically independent. Higher order Taylor series expansion could be used, along with higher-order statistical moments, to evaluate correlated variables, but that is beyond the scope of this paper.

Many mathematics texts address Taylor series expansion. Rather than presenting an inordinate amount of detail, only the results of the expansion process will be presented (Ang and Tang, 1975, Hahn and Shapiro, 1967). The expected value and the variance of the system equation above are:

$$E(S) = g[E(x_1), E(x_2), \ldots, E(x_n)] + \frac{1}{2}\sum_{i=1}^{n}\frac{\partial^2 g(x)}{\partial x_i^2} Var(x_i) + higher\ order\ terms \qquad \textbf{(6)}$$

$$Var(S) = \sum_{i=1}^{n}\left(\frac{\partial g(x)}{\partial x_i}\right)^2 Var(x_i) + higher\ order\ terms \ . \qquad \textbf{(7)}$$

The first moment or expected value of the system equation is a function of only two terms (to second order accuracy). The first term is the standard point estimate (simply evaluate the function using the mean values). The second term is a summation of the second partial derivatives of the system equation multiplied by the respective variances. After obtaining the partial derivative term, it is evaluated using the mean value for the variables in the derivative term. Occasionally, this term is displayed with symbolism signifying that the derivative should be evaluated at the mean values, but it is not used here for purposes of clarity.

The second moment or variance of the system equation is a function of only one term (to second order accuracy). This term is a summation of the first derivative squared multiplied by the respective variance. Once again, after the derivative term is evaluated, the mean values for the variables should be used to get a numerical result.

Since the two moments will be calculated numerically by using a spreadsheet, several mathematical operations must be performed, including multiplications, additions, and derivations. A spreadsheet is an ideal method for executing the first two operations, but it is not ideally suited for differentiation. While functionally simple, taking the numerical derivative of an equation and achieving reasonable results is sometimes difficult.

The derivative terms may be evaluated using standard numerical differentiation. From finite difference calculus, it can be shown (Hornbeck, 1975) that a central difference representation for the first and second derivative is:

$$\frac{\partial g(x_i)}{\partial x_i} \approx \frac{g_{i-2} - 8g_{i-1} + 8g_{i+1} - g_{i+2}}{12\Delta} \tag{8}$$

$$\frac{\partial^2 g(x_i)}{\partial x_i^2} \approx \frac{-g_{i-2} + 16g_{i-1} - 30g_i + 16g_{i+1} - g_{i+2}}{12\Delta^2} \quad , \tag{9}$$

where Δ is the mesh spacing or stepsize, g_{i-2} signifies the function g evaluated at x-2Δ, g_{i-1} signifies the function g evaluated at x-Δ, etc.

These two equations are accurate to the fourth order (Δ^4). But, if the stepsize is chosen too small such that calculations approach the accuracy of the computer's internal precision, additional inaccuracies may arise. Also, if the stepsize is chosen too large, the derivative equations will not produce accurate results due to the mesh size spanning too much of the evaluated function.

The question of what stepsize an analyst should use to perform the calculations may arise. One potential solution to the answer would be to vary the stepsize and check for convergence of the results. As a general starting point, I use a stepsize of 0.005. It should be pointed out that the stepsize used (e.g., 0.005) in the TSE spreadsheet is a multiplier on the mean values for the model parameters. Consequently, models containing variables with large mean values (e.g., 100,000,000) will use the same stepsize as models containing varialbe with small mean values (e.g., 0.0001).

Now that the derivative term has been defined, the tools are available to construct the Taylor series expansion spreadsheet. For the remainder of the paper, I will call the completed spreadsheet TSE. The TSE can be executed on any spreadsheet program that has a macro language. For the example presented in this paper, the TSE will be constructed using LOTUS 1-2-3, Release 3.1. The spreadsheet is designed such that the input/output screen is on worksheet A, while the macros are on worksheet B. For non-multidimensional spreadsheets, such as LOTUS 1-2-3, Release 2.x, minor translations (changing all "B" worksheet references to the "A" worksheet) will be necessary.

The overall layout of the spreadsheet is given in Figure 1. The spreadsheet must be built exactly as shown in order for the macros, ranges, and formulae to work correctly. The graphical lines and shading on the spreadsheet are not needed and are used only for illustrative purposes. The text shown in Figure 1 (such as "# variates", "Function =", etc.) are input as text labels in their appropriate cells.

The shaded areas in Figure 1 denote cells which require some type of input for the TSE to operate. Conversely, the unshaded cells could be locked to prevent user manipulations after the TSE design is complete.

The first shaded cell, B1, contains the total number of variates (or variables) in the function that is to be evaluated. The total number of variates corresponds to the subscript n in Equation 5. In theory, the total number of variates could be very large, but the TSE is designed such that a maximum of 15 variates should be used. A method of avoiding the 15 variate limit is discussed below.

The second shaded cell, E1, represents the actual function that is to be evaluated. The equation should be entered as a function of cells B4-B18, with B4 representing the first variate, B5 representing the second variate, B6 representing the third variate, etc. For example, if we wanted to examine the uncertainty of the distance x in the equation $x = vt + \frac{1}{2}at^2$, the function that would be entered into cell E1 would be ((B4*B5)+(.5*B6*(B5^2))), where cell B4 represents the velocity v, cell B5 represents the time t, and cell B6 represents the acceleration a.

The third shaded area corresponds to the variates discussed above. The cell range B4..C15 contains the mean and standard deviation for the variates contained in the function listed in cell E1. Thus, for the example in the previous paragraph, cell B4 would contain the mean value for the velocity while cell C4 would contain the velocity standard deviation value. Cell B5 contains the time mean value while the cell C5 would contain the time standard deviation value, and so on. It was stated above that the maximum number of variates is set at 15. To increase this maximum, continue listing the variate (16, 17, etc.) parameters down columns B and C. Also, the two defined ranges SUM1 and SUM2 (see Figure 4) need to be changed from A:H4..A:H18 and A:I4..A:I18 to A:H4..A:Hx and A:I4..A:Ix, respectively, where x denotes the total number of variates plus three. As an example, if the function had 25 variates, the range SUM1 would be A:H4..A:H28 while the range SUM2 would be A:I4..A:I28.

The last shaded area corresponds to the stepsize, which is represented by the Δ in Equations 8 and 9. As discussed, I routinely use a stepsize of 0.005. But, for most analyses, several values of the stepsize could be used to evaluate the effect of the value on the overall results. Also, the TSE could be modified so that the stepsize is automatically changed and the results printed or plotted for each stepsize value.

Now that the basic interface structure has been discussed, the macros, cell functions, and ranges will be discussed. First, the macro structure is contained in five separate macro functions. Figure 2 lists the TSE macros, all of which are contained on the B worksheet.

As shown in Figure 2, the five macros are listed in column B, while the macro description is listed in column A. Thus, the \R macro is typed into cells B2 to B3 as shown. After the macro is typed into the cells, the two cells must be named \R by using the Lotus range name command \RNC. When using Lotus 1-2-3, naming a macro with a backslash (\) then a letter allows the macro to be executed by pressing the letter while holding down the ALT key. Thus, TSE is executed by pressing R while the ALT key is depressed. The analysis should not be started until after entering the number of variates, the function, the variate's mean and standard deviation, and the stepsize.

Next, the cell functions need to be entered into the spreadsheet. Figure 3 shows the seven functions that must be entered and their respective cells. For cell A:E1 (cell E1 on worksheet A), the function to be entered is the user function. Thus, when first developing the TSE model, this cell should be left blank. The remainder of the functions should be entered as shown. The function for cell E22 appears to wrap around to a second line, but it should be entered as one continuous line in the cell.

And last, the worksheet ranges must be named. Figure 4 shows the range name and the cell range. All of the listed ranges should be named according to the list. For example, cell A:E21 should be named FIRST using the Lotus \RNC command. The bottom five ranges in the list are the macro ranges and should have been named previously when the macros were entered.

After the ranges are named, the TSE spreadsheet is complete and should be saved before using it for the first time. The example problem discussed below should be entered to help ensure that the spreadsheet was entered correctly. If the results are not identical to those presented, the macros and ranges should be carefully checked. But, if a different spreadsheet program is used (e.g., Quatro Pro or Excel), calculational or roundoff differences between the two program versions may result in slightly different results for the example problem.

4.0 Example Problem

For the sample problem to demonstrate the TSE, a problem from Hahn and Shapiro's (1967) statistics text was evaluated. The problem is to calculate the electron current for the circuit given in Figure 5. The equation to calculate the current in this circuit is:

$$I = V\left(\frac{1}{R_A} + \frac{1}{R_B} + \frac{1}{R_C}\right) \tag{10}$$

where I = the current (amps), V = the voltage potential (volts), and R = the resistance (ohms).

Each of these parameters is treated as a random variable. Each variable has an associated uncertainty. Since TSE only requires a mean and standard deviation, no distributional requirements are imposed on the analysis. Such requirements would be needed if Monte Carlo analysis were employed to solve the problem.

Table 1 lists each variate in the circuit equation with its mean and standard deviation. All variates are assumed to be mutually statistically independent since the independence assumption was used in the TSE development. The values in Table 1 were put into the spreadsheet and the TSE macros were executed by pressing the R key while the ALT key is depressed. Figure 6 shows the order of steps and the cell input at each step taken to evaluate the circuit equation.

Table 1. Variate parameters for the TSE example problem.

Variate	Mean	Standard Deviation
V	120	3.8730
R_A	10	1.0
R_B	15	1.0
R_C	20	1.4142

The TSE spreadsheet gives the following results for the circuit problem: point estimate = 26, mean = 26.18555, and standard deviation = 1.61512. Hahn and Shapiro gave the second-order, "hand calculated" (e.g., analytical derivatives rather than numerical derivatives) answers for the electron current as: mean = 26.19, and standard deviation = 1.6155. For this paper, a Monte Carlo analysis was also performed for the circuit problem. Each random variate was assumed to be normally distributed with mean and standard deviation given in Table 1. For a sample of size 4000, the mean = 26.190 and the standard deviation = 1.683.

As can be seen above, the TSE spreadsheet gives consistent answers for both the hand calculated results and the Monte Carlo simulation. Even though the electron current equation is nonlinear (with respect to the resistance), the Taylor series analysis agrees with the Monte Carlo simulation.

5. Conclusions and Considerations

The TSE spreadsheet evaluates the statistical uncertainty in functions of up to 15 variables. This paper guides the reader through setting up the TSE spreadsheet and using the completed spreadsheet to evaluate equations consisting of random variables. As illustrated in the example problem, TSE can accurately calculate the uncertainty for some non-linear functions (e.g., equation 10).

Someone with experience in using electronic spreadsheets should be able to use the provided spreadsheet layout, macros, cell functions, and range names to analyze the uncertainty for a user-supplied formula. Although the user-supplied formula is restricted to 15 random variables, a method of bypassing this variable limit is furnished.

While it was shown that the TSE spreadsheet does perform well, situations may arise where the Taylor series expansion analysis will differ significantly from Monte Carlo analysis. Usually, this situation occurs only when the evaluated function is nonlinear or contains distributions which are highly skewed. If the Monte Carlo analysis parameters have highly skewed distributions, the Taylor series analysis may not adequately model the parameter variability (because higher order terms are needed, additional derivations to the TSE equation are required, and moment estimators for the higher order terms are frequently poor).

Increasing the TSE analysis to a higher order (third or fourth order) may eliminate some of the discrepancies between Monte Carlo and Taylor series analysis; that, however, is beyond the scope of this paper. Regardless, the reader may find that the second-order TSE analysis presented in this paper is adequate for many uncertainty analysis problems. Also, the TSE analysis could provide a quick verification of a model that was exclusively analyzed by Monte Carlo simulation, providing the equation for the model is known.

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	A	B	C	D	E	F	G	H	I
1	# variates			Function =					
2									
3	Variate	Mean	Std. dev.	F R	Point estimate			Sum1	Sum2
4	1			U E					
5	2			N S					
6	3			C U	Expected value				
7	4			T L					
8	5			I T					
9	6			O S	Std. deviation				
10	7			N					
11	8								
12	9								
13	10			oldmean =		F1=			
14	11			I =		F2=			
15	12			H =		F3=			
16	13			stepsize =		F4=			
17	14			J =		F5=			
18	15			tempmean=					
19									
20				variance =					
21				1st dir. =					
22				2nd dir. =					

Figure 1. TSE spreadsheet layout.

B:	A	B
1		
2	\R	/wgpd{windowsoff}{FOR i,1,n-1,1,tse}{tse}
3		{results}{calc}{windowson}/wgpe
4		
5	TSE	{for J,1,4,1,loop}{loop}{math}
6		
7	LOOP	{calc}{let @coord(1,2,I+3,1),tempmean}
8		{recalccol function}{let @coord(1,7,j+12,1),function}
9		{let @coord(1,2,i+3,1),oldmean}
10		
11	MATH	{calc}{let @coord(1,8,i+3,1),$A:$E$21}
12		{let @coord(1,9,i+3,1),$A:$E$22}
13		
14	RESULTS	{let $A:$E$7,($A:$E$4)+@sum(sum2)}
15		{let $A:$E$10,+@sqrt(@sum(sum1))}

Figure 2. TSE macro commands (worksheet B).

CELL	FUNCTION
A:E1	*user defined function*
A:E4	+$E$1
A:E13	@@(@COORD(1,2,I+3,1))
A:E15	(OLDMEAN*STEPSIZE)
A:E18	(OLDMEAN+((J-3)*H))
A:E20	(@@(@COORD(1,3,I+3,1)))^2
A:E21	(VARIANCE*((FUNC1-(8*FUNC2)+(8*FUNC4)-FUNC5)/(12*H))^2)
A:E22	(1/2)*(VARIANCE)*(-FUNC1+(16*FUNC2)-(30*FUNC3)+(16*FUNC4) -FUNC5)/(12*H^2))

Figure 3. TSE cell functions.

NAME	RANGE
FIRST	A:E21
FUNC1	A:G13
FUNC2	A:G14
FUNC3	A:G15
FUNC4	A:G16
FUNC5	A:G17
FUNCTION	A:E1
H	A:E15
I	A:E14
J	A:E17
N	A:B1
OLDMEAN	A:E13
SECOND	A:E22
STEPSIZE	A:E16
SUM1	A:H4..A:H18
SUM2	A:I4..A:I18
TEMPMEAN	A:E18
VARIANCE	A:E20
\R	B:B2..B:B3
TSE	B:B5
LOOP	B:B7..B:B9
MATH	B:B11..B:B12
RESULTS	B:B14..B:B15

Figure 4. TSE defined ranges

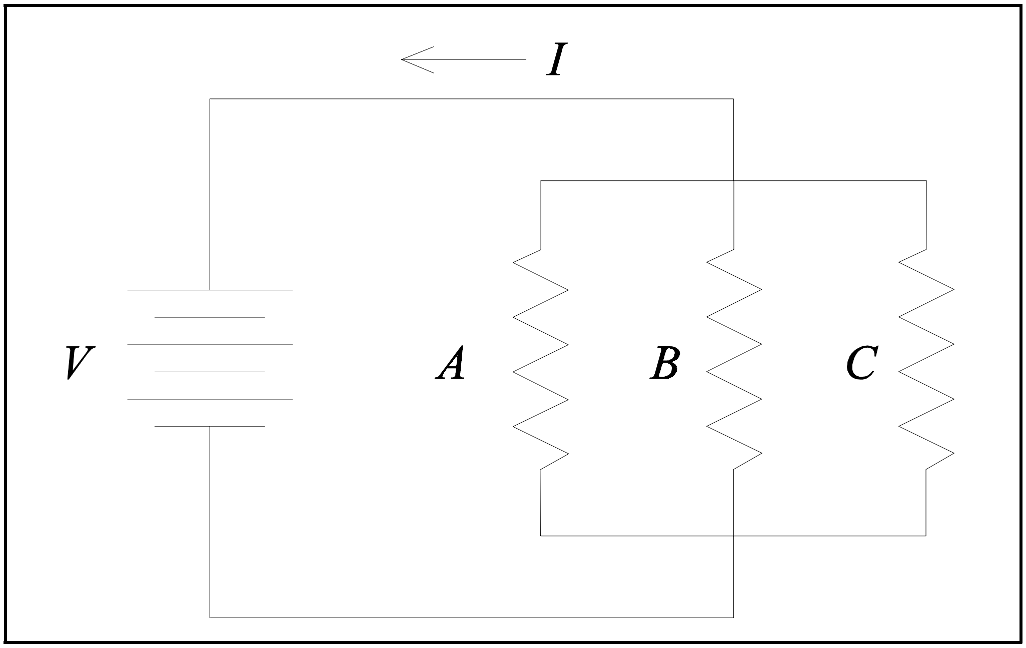

Figure 5. Circuit diagram for the TSE example problem.

Cell	Input	Comment[a]
B1	4	The total number of variates
B4	120	Voltage mean
C4	3.873	Voltage standard deviation
B5	10	Resistance A mean
C5	1	Resistance A standard deviation
B6	15	Resistance B mean
C6	1	Resistance B standard deviation
B7	20	Resistance C mean
C7	1.4142	Resistance C standard deviation
E1	+B4*((1/B5)+(1/B6)+(1/B7))	Circuit Equation

Start macro by pressing Alt-R

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[a] The comments are not input to the spreadsheet and are for instructional purposes only.

Figure 6. Circuit problem input steps.